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ORIGINAL PAPER

A probabilistic evolution approach trilogy, part 1: quantum expectation value evolutions, block triangularity and conicality, truncation approximants and their convergence

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Abstract This is the first one of three companion papers focusing on the “probabilistic evolution approach (PEA)” which has been developed for the solution of the explicit ODE involving problems under certain consistent impositions. The main purpose here is the determination of the expectation value of a given operator in quantum mechanics by solving only ODEs, not directly using the wave function. To this end we first define a basis operator set over the Kronecker powers of an appropriately defined “system operator vector”. We assume that the target operator’s commutator with the system’s Hamiltonian can be expressed in terms of the above-mentioned basis operators. This assumption leads us to an infinite set of linear homogeneous ODEs over the expectation values of the basis operators. Its coefficient matrix is in block Hessenberg form when the target operator has no singularity, and beyond that, it may become block triangular when certain conditions over the system’s potential function are satisfied. The initial conditions are the basic determining agents giving the probabilistic nature to the solutions of the obtained infinite set of ODEs. They may or may not have fluctuations depending on the nature of the probability density. All these issues are investigated in a phenomenological and constructive theoretical manner in this paper. The remaining two papers are devoted to further details of PEA in quantum mechanics, and, the application of PEA to systems defined by Liouville equation.

Keywords Probabilistic evolution · Expectation value dynamics · Evolution matrices · Block triangularity · Conicality · Initial conditions and fluctuations

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1 Introduction

The “probabilistic evolution approach (PEA)”, which has been proposed and developed up to a certain level of maturity by Metin Demiralp and partially by his colleagues, presents a way of obtaining an infinite linear ODE set for any given explicit ODE set whose right hand side functions, which may be called “descriptive functions”, are assumed not to depend explicitly on time. This autonomy is not a generality loss since by defining a new extra unknown identically the same as the time variable brings the autonomy if it does not exist. In PEA, we consider a Kronecker power basis set whose elements are the products of the nonnegative integer powers of the terms defining the deviations of the unknowns from given constant target values (expansion point components). Hence, this basis set elements depend on time and this urges us to construct an ODE for each basis element. We use certain well-known features of the Kronecker product and the matrix–matrix, and/or, matrix-vector products together with the given set of explicit ODEs to get a denumerably infinite number of ODEs which are first order, linear, homogeneous and with an infinite constant coefficient matrix which we call “evolution matrix” since it is completely responsible for the evolution of an initial state to another state at a specified time instance. The evolution matrix is in upper block Hessenberg form unless its descriptive functions vanish at the expansion point which is in the linear vector space (state space, phase space), then it becomes block triangular. Of course the block triangularity facilitates the analysis very much especially in the sense of spectral issues. The vanishing property may or may not exist in the descriptive functions or it may exist more than once. What we know from the PEA is that the truncated solutions obtained from the upperleftmost of the infinite equations converge to the actual solution as long as the initial data points to a location remaining inside the complex plane disk (or the complex space hypersphere in the case of multivariance) centered at the expansion point and excluding the nearest zero point of the descriptive functions. Hence, in the case of single zero one can expect convergence for entire complex plane (or complex space in the case of multivariance) which excludes the complex infinity. On the other hand the case where there appears more than one zero in the descriptive functions expansion point can be chosen as one of these zero points and each choice produces a different but intersecting finite convergence domains. The union of these regions defines the total finite region of convergence, outside which can be brought to the utilization by using certain inverse type functionalities like it is done in the analytic continuations of the conventional complex analysis.

We intend to deal mostly with entire (or integer in an equivalent naming) functions for facilitating analysis. This does not in fact restrict the analysis since for all other type descriptive functions even the ones with the singularities, the considered set of ODEs can be principally converted to another ODE set with entire descriptive functions by adding new appropriate unknowns in terms of standing ones and therefore increasing the dimensionality of the exist ing state space. We call this procedure “space extension” and it moves all the singular functionalities from the ODE structures to the initial conditions or some other impositions.

The space extension enables the ODE set to gain conicality, that is, having at most second degree multinomiality in the descriptive functions. The conicality is reflected to the evolution matrix as the block diagonal structure composed of the main diagonal and its nearest upper and lower diagonal neighbors. If the expansion point is chosen so that the descriptive functions vanish there then all the lower nearest diagonal blocks of the evolution matrix vanish. This enables us to separate the total infinite set of equations to infinite number of finite block ODEs each of which is one of the elements of a first order recursion whose analytic solution can be formally constructed, and, the truncation approximants can be rather easily constructed.

Now we are sufficiently motivated and encouraged to extend PEA to physically true probabilistic systems. The quantum systems (probability arises from the difference in scales of macro and micro systems) described by the Schrödinger equations and the statistical systems (probability arises from the unmanageably high numbers of freedom). This paper and its next companion are devoted to the first one of the systems while the last paper of this trilogy makes a gentle introduction to the PEA application for the latter case.

If we skip Heisenberg's Matrix Formalism and follow the Schrödinger's Wave Equation Formalism then the determination of the wave function becomes the main focus of the quantum dynamical problems even though the wave function is not needed directly to evaluate the observables. The known wave function means that any observable which can be defined through an appropriate operator's expectation value can be evaluated in principle. However, this is not so mandatory as it appears. The wave function can be bypassed by formulating ordinary differential equations whose unknowns are the certain expectation values which can be directly considered as temporal entities. In the cases focusing on the evaluation of the wave function, the time-dependent Schrödinger equation's solution becomes the main target. This equation is a linear partial differential equation having parabolic and elliptic natures in time and spatial coordinates, respectively. The parabolic temporal behaviour urges us to give the initial wave form while the ellipticity is accompanied by certain boundary conditions designed in accordance with the physics of the system under consideration (it is not compulsory to give boundary conditions for ellipticity, the initial value problems like Cauchy problems can also be designed, but this is not a frequently encountered issue in the world of quantum physics). The solution of the Schrödinger equation completely depends on how simple its Hamiltonian structure is. The analytically solvable cases are quite rare and the numerical solutions may become formidable when the system's degree of freedom climbs up to higher numbers. Hence, special methods were developed to approximate the solution for special group of systems. All these urge us to develop a method to find the observable values without solving the Schrödinger's equation.

Our main goal is to write down the expectation value of a given operator expressed in fundamental system operators like positions and momenta and then to obtain an ODE via simple temporal differentiation followed by the evaluation of the operator's commutator with system's Hamiltonian. This produces new expectation values over new operators arising from the commutation of the operator with the system Hamiltonian and urges us to construct new ODEs. However, this procedure may result in infinite number of ODEs unless the given operator and the system Hamiltonian lie in a finite set of operators, which is closed under the commutation operation with the system Hamiltonian. Finite or infinite, the resulting set of ODEs are first order and can be accompanied by certain initial values of the relevant operators' expected values. These initial value impositions do not require the wave function but its initial form which is not to be evaluated but to be given. Hence this procedure bypasses the evaluation of the wave function. Our main task here is the construction of an expectation value dynamics over certain universal entities which do not depend on the target operator but depends only on system entities.

2 Quantum expectation dynamical equations

Let us consider the time dependent Schrödinger's equation given in the following closed form

$$i\hbar \frac{\partial \psi\left(\mathbf{x}, t\right)}{\partial t} = \widehat{H}\psi(\mathbf{x}, t), \quad \psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}) \tag{1}$$

where t and $\mathbf{x}$ stand for time and spatial coordinates, respectively while the explicit structure of the Hamiltonian operator is not given even though its dependence on momenta is limited to the second degree multinomiality. For the derivation of the equations of motion in expectation values we do not need this explicity in fact. The expectation or expected value of a given operator $\widehat{O}$ is defined as

$$\left\langle \widehat{O} \right\rangle(t) \equiv \int_V dV \psi\left(\mathbf{x}, t\right)^* \widehat{O} \psi\left(\mathbf{x}, t\right) \tag{2}$$

where V and dV denote the integration domain over spatial variables and infinitesimal volume element of integration, respectively while the superscript star means complex conjugation. So expectation value of any given operator can vary only in time. Even though it is possible to deal with time variant operators we focus on time independent operators here since they suffice for our present purposes.

The temporal differentiation of both sides of (2) produces a new integral at the right hand side such that the integrand contains the time derivatives of the wave function and its complex conjugate. These temporal derivatives can be expressed in images of the relevant functions under the Hamilton operator. The right hand side integral can also be considered as an inner product. The Hermiticity of the Hamilton operator enables us to transfer the action of the Hamiltonian on the wave function's complex conjugate to the other part of the integrand. All these urge us to write the following equality

$$\begin{aligned} \frac{d\left\langle \widehat{O} \right\rangle(t)}{dt} &= \int_V dV \psi\left(\mathbf{x}, t\right)^* \left\{ \frac{i}{\hbar} \left[\widehat{H}\widehat{O} - \widehat{O}\widehat{H} \right] \right\} \psi\left(\mathbf{x}, t\right) \\ &= \left\langle \frac{i}{\hbar} \left[\widehat{H}\widehat{O} - \widehat{O}\widehat{H} \right] \right\rangle(t) \end{aligned} \tag{3}$$

The accompanying initial condition to this ODE can be given as follows

$$\left\langle \widehat{O} \right\rangle(0) \equiv \int_V dV \psi_0\left(\mathbf{x}\right)^* \widehat{O} \psi_0\left(\mathbf{x}\right). \tag{4}$$

(3) and (4) become meaningful and practical if the expected value of the commutator between the system Hamiltonian and the operator $\widehat{O}$ can be expressed in terms of the expected value of $\widehat{O}$. Otherwise we need to define a new operator as follows

$$\widehat{O}_1 \equiv \frac{i}{\hbar}\left[\widehat{H}\widehat{O} - \widehat{O}\widehat{H}\right] \tag{5}$$

and then try to obtain a new ODE over the expected value of this operator. However, this may produce a new commutator enforcing us to define a new operator $\widehat{O}_2$ and therefore urging us to construct another ODE. This procedure may never end unless one of the commutators can be expressed as a linear combination of the operators appearing up to that point. This issue is related to commutator algebra and therefore Lie Algebra. However, we do not intend to proceed in this direction here since we do not actually need it.

An important issue here is the autonomy in the Hamiltonian. If the system under consideration is isolated from its environment then the system's behaviour is reflected to the Hamiltonian via certain time invariant entities like kinetic energy operator and potential function. On the other hand the systems under external influences can be described only via time dependent Hamiltonian unless the external field has a very specific nature. Here, in this work, we assume autonomy in the Hamiltonian to facilitate the analysis. What we obtain here can be extended to nonautonomous cases without having any serious difficulties. To this end, certain space extension methods can be used.

3 Probabilistic evolution equations (PEEs)

The fundamental entities characterizing a quantum system are basically momentum and position operators and the system Hamiltonian also depends on these entities. These entities can be considered as the elements of a Cartesian vector we call "state vector" or "system vector". However, we do not intend to emphasize on the discrimination of the state characterizing entities like positions and momenta. We write the state vector as follows

$$\mathbf{s} \equiv \left[\,\widehat{s}_1 \;\ldots\; \widehat{s}_n\,\right]^T \tag{6}$$

where n stands for the "system's dimension". This is twice the degree of the freedom for the considered system. The s elements can be called "state operators". They may be position or momentum operators in many practical cases. The important issue for the analysis here is not their specific nature but the nature of the general operator.

The state vector's Kronecker square (Kronecker product with itself) is explicitly defined as follows

$$\mathbf{s}^{\otimes 2} \equiv \mathbf{s} \otimes \mathbf{s} \equiv \left[\, s_1 \mathbf{s}^T \;\ldots\; s_n \mathbf{s}^T \,\right]^T \tag{7}$$

which can be generalized to the following general formula

$$\mathbf{s}^{\otimes m} \equiv \mathbf{s} \otimes \mathbf{s}^{\otimes (m-1)} \equiv \left[\, s_1 \mathbf{s}^{\otimes (m-1)^T} \;\ldots\; s_n \mathbf{s}^{\otimes (m-1)^T} \,\right]^T, \quad m = 1, 2, 3, \ldots \tag{8}$$

where n^m number of elements exist in the mth Kronecker power of the state vector. Even though this formula is given for positive integer Kronecker powers it can also be extended to zeroth Kronecker power by following the traditional approaches in the similar area. We define the zeroth Kronecker power as the universal scalar operator, just the identity operator (in other words it is a single element vector).

The expectation value of the state vector can be expressed as follows

$$\frac{d\left\langle \mathbf{s}\right\rangle (t)}{dt}=\left\langle \frac{i}{\hbar}\left[\,\widehat{H}\widehat{\mathbf{s}}-\widehat{\mathbf{s}}\widehat{H}\,\right]\right\rangle (t) \tag{9}$$

At this point we need to assume some structure for the right hand side of this equation. By taking the inspirations from the analytic functions and Taylor series we can assume the following infinite series representation

$$\frac{i}{\hbar}\left[\,\widehat{H}\widehat{\mathbf{s}}-\widehat{\mathbf{s}}\widehat{H}\,\right]\equiv\sum_{j=0}^{\infty}\mathbf{H}_j\mathbf{s}^{\otimes j} \tag{10}$$

where $\mathbf{H}_j$ is a constant matrix of $n\times n^j$ type, depending on and therefore characterizing the system under consideration. The insertion of this assumption to the right hand side of (9) produces

$$\frac{d\left\langle \mathbf{s}\right\rangle (t)}{dt}=\sum_{j=0}^{\infty}\mathbf{H}_j\left\langle \mathbf{s}^{\otimes j}\right\rangle (t) \tag{11}$$

which urges us to evaluate the expectation value of the mth Kronecker power of the state vector. To this end we can start by writing the following identity

$$\widehat{H}\widehat{s}_j\widehat{s}_k-\widehat{s}_j\widehat{s}_k\widehat{H}\equiv\left[\,\widehat{H}\widehat{s}_j-\widehat{s}_j\widehat{H}\,\right]\widehat{s}_k+\widehat{s}_j\left[\,\widehat{H}\widehat{s}_k-\widehat{s}_k\widehat{H}\,\right] \tag{12}$$

which states that the commutation operation is distributed over the binary products by paying sufficient care to the multiplication order. This is somehow identical to the Leibniz rule for differentiation over binary products. This distributive identity is not peculiar only to binary products but it can be extended to any product involving more than two factors. We can immediately adapt this identity to a binary Kronecker product and write the following identity

$$\widehat{H}\mathbf{s}\otimes\mathbf{s}-\mathbf{s}\otimes\mathbf{s}\widehat{H}\equiv\left[\,\widehat{H}\mathbf{s}-\mathbf{s}\widehat{H}\,\right]\otimes\mathbf{s}+\mathbf{s}\otimes\left[\,\widehat{H}\mathbf{s}-\mathbf{s}\widehat{H}\,\right] \tag{13}$$

which can be generalized to the Kronecker powers of the state vector as follows

$$\widehat{H}\mathbf{s}^{\otimes j}-\mathbf{s}^{\otimes j}\widehat{H}\equiv\sum_{k=0}^{j-1}\mathbf{s}^{\otimes k}\otimes\left[\,\widehat{H}\mathbf{s}-\mathbf{s}\widehat{H}\,\right]\otimes\mathbf{s}^{\otimes(j-1-k)}. \tag{14}$$

This result can be combined with (10) to obtain

$$\frac{i}{\hbar}\left[\widehat{H}\mathbf{s}^{\otimes j}-\mathbf{s}^{\otimes j}\widehat{H}\right]\equiv\sum_{\ell=0}^{\infty}\sum_{k=0}^{j-1}\mathbf{s}^{\otimes k}\otimes\mathbf{H}_{\ell}\mathbf{s}^{\otimes\ell}\otimes\mathbf{s}^{\otimes(j-1-k)}\tag{15}$$

where we can use the following identities if $\mathbf{I}_n$ stands for the $n\times n$ identity matrix

$$\begin{aligned}\mathbf{s}^{\otimes k}&\equiv\mathbf{I}_n^{\otimes k}\mathbf{s}^{\otimes k}\\ \mathbf{s}^{\otimes k}\otimes\mathbf{H}_{\ell}\mathbf{s}^{\otimes\ell}\otimes\mathbf{s}^{\otimes(j-1-k)}&\equiv\left[\mathbf{I}_n^{\otimes k}\otimes\mathbf{H}_{\ell}\otimes\mathbf{I}_n^{\otimes(j-1-k)}\right]\mathbf{s}^{\otimes(j-1+\ell)}\end{aligned}\tag{16}$$

the last one of which is derived by using the mutually distributive property of the matrix products and outer products.

If we define

$$\mathbf{E}_{j,j+\ell-1}\equiv\sum_{k=0}^{j-1}\mathbf{I}_n^{\otimes k}\otimes\mathbf{H}_{\ell}\otimes\mathbf{I}_n^{\otimes(j-1-k)}\tag{17}$$

then we can rewrite (15) as follows

$$\frac{i}{\hbar}\left[\widehat{H}\mathbf{s}^{\otimes j}-\mathbf{s}^{\otimes j}\widehat{H}\right]\equiv\sum_{\ell=0}^{\infty}\mathbf{E}_{j,\ell}\mathbf{s}^{\otimes\ell}\tag{18}$$

which allows us to write

$$\frac{d\left\langle\mathbf{s}^{\otimes j}\right\rangle(t)}{dt}=\sum_{\ell=0}^{\infty}\mathbf{E}_{j,\ell}\left\langle\mathbf{s}^{\otimes\ell}\right\rangle(t),\quad j=0,1,2,\ldots\tag{19}$$

These denumerably infinite number of the equations can be put in to a more concise form by defining

$$\boldsymbol{\xi}(t)\equiv\left[\left\langle\mathbf{s}^{\otimes 0}\right\rangle(t)^{T}\ \left\langle\mathbf{s}^{\otimes 1}\right\rangle(t)^{T}\ \ldots\right]^{T}\tag{20}$$

$$\mathbf{E}\equiv\begin{bmatrix}\mathbf{E}_{0,0}&\cdots&\mathbf{E}_{0,m}&\cdots\\ \vdots&\ddots&\vdots&\vdots\\ \mathbf{E}_{m,0}&\cdots&\mathbf{E}_{m,m}&\cdots\\ \vdots&\vdots&\vdots&\ddots\end{bmatrix}\tag{21}$$

which urge us to write

$$\frac{d\boldsymbol{\xi}(t)}{dt}=\mathbf{E}\boldsymbol{\xi}(t)\tag{22}$$

As can be immediately noticed the constant infinite matrix $\mathbf{E}$'s first row is composed of only zeroes while the other block rows have dimensions n, n^2, n^3, and so on. This block structure is in such a way that all lower diagonal blocks except the ones residing in the closest neighbour of the main diagonal blocks vanish. This means that $\mathbf{E}$ is in upper block Hessenberg form. This may bring a lot of advantages. However, it is better to have triangular form for practicality. Triangularity may avail only when $\mathbf{H}_0$ which is an n-element vector vanishes. The survival of this property is peculiar to the system under consideration and to how the state vector is defined. Its definition can be changed even preserving the dependence on the same operators, by using certain functional relations like affine transformations.

The constancy of the matrix $\mathbf{E}$, we call "evolution matrix" since it is responsible for the expectation value system's general behaviour not depending on the initial conditions, enables us to write the formal solution of (22) as follows

$$\boldsymbol{\xi}(t) = \mathrm{e}^{t\mathbf{E}}\boldsymbol{\xi}(0) \tag{23}$$

The second block which is an n element vector gives the expectation values of the state operator as a function of time. The other blocks are also meaningful. They can be used to evaluate the mathematical fluctuations in the expectation values. For example, the third block is the expectation value of the Kronecker square of the state vector and we can not expect its equality to the Kronecker square of the expectation value of the state vector unless the initial wave form is sharply localized like Dirac delta function. In a crude statement, the expectation value of the square of an operator is not equal to the square of the expectation value of the same operator in the nonexistence of sharply localized probability distributions. The statement can be extended to higher Kronecker powers accordingly and each of them can be used to define a different and separate mathematical fluctuation.

4 Block triangularity and truncation approximants

As we mentioned above the n-element vector $\mathbf{H}_0$ is responsible for making the evolution matrix block triangular. In many cases the state vector is composed of momentum and position operators and the Hamiltonian is such that this vector vanishes if the vector of position coordinates, $\mathbf{x}$ resides at a minimum of the potential function of the system because some of its elements like momenta spontaneously vanish while the others are the partial derivatives of the potential function evaluated at the origin if xs themselves are taken as some of the s elements. The origin may not be a minimum of the potential function. Then the definitions of ss may be changed to the powers of shifted values of the x coordinates to match a minimum of the potential. Thus $\mathbf{H}_0$ is made to vanish. However, this is true for the potential functions whose values at their minima are finite. Otherwise there are certain singularities in the potential and all the above analysis fails. We do not consider these cases here but leave them to another paper of our group. So what we can say about block triangularity is that it can be provided by working with powers of the differences in spatial coordinates from a specific point in the position space of the system under consideration.

Once the block triangularity is provided; the next step is to truncate the probabilistic evolution equations from its left uppermost part as follows

$$\boldsymbol{\xi}_{n_t}(t) \equiv \left[\left\langle \mathbf{s}^{\otimes 0} \right\rangle (t)^T \left\langle \mathbf{s}^{\otimes 1} \right\rangle (t)^T \ldots \left\langle \mathbf{s}^{\otimes n_t} \right\rangle (t)^T \right]^T \tag{24}$$

$$\mathbf{E}_{n_t} \equiv \begin{bmatrix} \mathbf{E}_{0,0} & \cdots & \mathbf{E}_{0,n_t} \\ \vdots & \ddots & \vdots \\ \mathbf{E}_{n_t,0} & \cdots & \mathbf{E}_{n_t,n_t} \end{bmatrix} \tag{25}$$

where n_t is a nonnegative integer defining the level of the truncation. The truncated evolution matrix $\mathbf{E}_{n_t}$ is upper block triangular since all its lower triangular blocks vanish. The probabilistic evolution equation now becomes

$$\frac{d\boldsymbol{\xi}_{n_t}(t)}{dt} = \mathbf{E}_{n_t} \boldsymbol{\xi}_{n_t}(t) \tag{26}$$

whose solution is given as follows

$$\boldsymbol{\xi}_{n_t}(t) = \mathrm{e}^{t\mathbf{E}_{n_t}} \boldsymbol{\xi}_{n_t}(0). \tag{27}$$

The block triangularity of (25) urges us to evaluate the diagonal blocks of the evolution matrix since their exponential functions gain great importance for the evaluation of the truncated solution. To this end we can write

$$\mathbf{E}_{j,j} \equiv \sum_{k=0}^{j-1} \mathbf{I}_n^{\otimes k} \otimes \mathbf{H}_1 \otimes \mathbf{I}_n^{\otimes (j-1-k)}, \quad j = 0, 1, 2, \ldots \tag{28}$$

whose summands are square type matrices which are also mutually commutative as can be shown by using the standard features of the Kronecker product. Therefore we can write

$$\mathrm{e}^{t\mathbf{E}_{j,j}} = \prod_{k=0}^{j-1} \mathrm{e}^{t\left[\mathbf{I}_n^{\otimes k} \otimes \mathbf{H}_1 \otimes \mathbf{I}_n^{\otimes (j-1-k)} \right]}, \quad j = 0, 1, 2, \ldots \tag{29}$$

where the argument of the exponential factors satisfy the following powering relations

$$\left[\mathbf{I}_n^{\otimes k} \otimes \mathbf{H}_1 \otimes \mathbf{I}_n^{\otimes (j-1-k)} \right]^m = \mathbf{I}_n^{\otimes k} \otimes \mathbf{H}_1^m \otimes \mathbf{I}_n^{\otimes (j-1-k)}, \quad j = 0, 1, 2, \ldots \tag{30}$$

which permit us to rewrite (29) as follows

$$\mathrm{e}^{t\mathbf{E}_{j,j}} = \prod_{k=0}^{j-1} \mathbf{I}_n^{\otimes k} \otimes \mathrm{e}^{t\mathbf{H}_1} \otimes \mathbf{I}_n^{\otimes (j-1-k)} = \left[\mathrm{e}^{t\mathbf{H}_1} \right]^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{31}$$

where the rightmost equation has been constructed by using the mutual distributive property of the matrix product and Kronecker product. We define

$$\mathbf{F}(t) \equiv e^{t\mathbf{H}_1}, \tag{32}$$

where $\mathbf{F}(t)$ is apparently $n \times n$ type time variant matrix. It characterizes the system's evolution since the truncated solutions' time variance comes purely from this entity. We call this matrix "fundamental propagator" of the system under consideration. As seen from above the time variance of the fundamental propagator is completely determined by $\mathbf{H}_1$. This is responsible for the stability of the system, that is, the behavior of the system when time grows unboundedly. Spectral decompositions of $\mathbf{H}_1$s can be used to get more explicit expressions for the fundamental propagator. Each element of fundamental propagator is a linear combination of the scalar exponential functions whose arguments are just time scaled by one of the eigenvalues of the relevant $\mathbf{H}_1$ matrix as long as the algebraic and geometric multiplicities in each eigenvalue are the same (otherwise the exponential functions may need to be multiplied by certain positive integer powers of t). Hence, the spectrum of $\mathbf{H}_j$ is solely responsible for the stability of $\mathbf{F}_j$ unless the algebraic and geometric multiplicities of eigenvalues differ. The spectrum is generally composed of pure imaginary numbers, by making the system behavior oscillatory. If this does not happen then the scattering phenomena which somehow corresponds to the singularities in the Hamiltonian is encountered. We do not intend to go beyond this point here since it exceeds the scope of the paper.

5 Conicality and space extension possibilities

The block triangularity is important because it removes many complications coming from the upper Hessenberg block form like the possibility of continuous spectrum appearance for the evolution matrix due to its infinite structure. However, it does not provide us with the simplest structure in the evolution matrix since full triangular structure complicates even the construction of truncated approximants. The best structure in the evolution matrix is of course the case of block diagonality which can not be obtained unless the system under consideration possesses very particular features. Beyond the diagonality, the simplest case is two banded structure in the evolution matrix (conicality in the descriptive functions). The conicality means that the commutator of the system Hamiltonian with the state vector can be expressed as a linear combination of the state vector and its Kronecker square if the evolution matrix is triangular, otherwise a constant vector is added. This may not be spontaneously happening unless certain specific characters exist in the system. This raises the question "is it possible to consider the system in an extended space which has a dimension greater than the original one?". The answer may not be "yes" in all circumstances. However, we have shown that the definition of new entities depending on the system variables and regarding them as new independent variables facilitates the construction of the probabilistic evolution equations to have an evolution matrix having nonvanishing blocks only on its main diagonal and its closest upper neighbor, (that is, in conical form).

In quantum mechanics the system characterizing agents are not just scalar entities but (at least partially, half of the entities) operators because of the existence of the momentum operators. As a matter of fact the position related entities can also be considered as the multiplication operators multiplying their operands by the corresponding spatial coordinates. However, unless the commutativity issues are on the stage, they can be represented by the corresponding spatial coordinates at the benefit of scalar utilization. The position dependent entities are generally potential functions whose structures determine how the space can be extended to get conicality. However, we do not intend to proceed further in this direction since it is out of the scope of this general theoretical presentation. The curious readers can refer to related publications of the author and his group, or, contact the author, himself.

6 Initial conditions and the probabilistic nature

We need now to focus on the initial conditions. To this end we can write

$$\boldsymbol{\xi}(0) \equiv \left[\left\langle \mathbf{s}^{\otimes 0} \right\rangle (0)^T \; \left\langle \mathbf{s}^{\otimes 1} \right\rangle (0)^T \; \ldots \right]^T \tag{33}$$

where

$$\left\langle \mathbf{s}^{\otimes m} \right\rangle (0) \equiv \int_V dV \psi_0 (\mathbf{x})^* \, \mathbf{s}^{\otimes m} \psi_0 (\mathbf{x}) \,, \quad m = 0, 1, 2, \ldots \tag{34}$$

which leads to the following inequality

$$\left\langle \mathbf{s}^{\otimes m} \right\rangle (0) \neq \langle \mathbf{s} \rangle (0)^{\otimes m}, \quad m = 0, 1, 2, \ldots \tag{35}$$

unless the probability density (complex modulus square of the initial wave form) becomes sharply localized at a point in the space spanned by $\mathbf{x}$. This inequality reflects the mathematical fluctuation in the mth Kronecker power of the state vector expected value. Therefore, as long as the probability distribution is not condensed at a single point there are unavoidable fluctuations in the initial values. In the case of no fluctuation the initial form of the $\boldsymbol{\xi}$ infinite vector becomes a power vector whose block elements are the nonnegative integer Kronecker powers of its second block. All these mean that the word "probabilistic" comes from this point and the probabilistic nature completely comes from the initial vector structure. In the case of probabilistic evolution for initial value problems of ODEs, the initial vector is a power vector and the probability density is like Dirac delta function. In the present case, the case for quantum mechanics, the probabilistic nature is reflected to the solutions through initial conditions and is created by the initial form of the wave function.

7 Convergence of the probabilistic evolution approach solutions

The expectation value of state vector's jth Kronecker power can be rewritten as follows when the evolution matrix is upper block triangular and having two adjacent diagonals, the main diagonal and its nearest upper neighbor

$$\frac{d\left\langle \mathbf{s}^{\otimes j}\right\rangle(t)}{dt} = \mathbf{E}_{j,j}\left\langle \mathbf{s}^{\otimes j}\right\rangle(t) + \mathbf{E}_{j,j+1}\left\langle \mathbf{s}^{\otimes(j+1)}\right\rangle(t), \quad j = 0, 1, 2, \ldots \tag{36}$$

which can be solved for the expectation value of the jth Kronecker power of the state vector as follows

$$\left\langle \mathbf{s}^{\otimes j}\right\rangle(t) = e^{t\mathbf{E}_{j,j}}\left\langle \mathbf{s}^{\otimes j}\right\rangle(0) + \int_0^t d\tau e^{(t-\tau)\mathbf{E}_{j,j}}\mathbf{E}_{j,j+1}\left\langle \mathbf{s}^{\otimes(j+1)}\right\rangle(\tau), \quad j = 0, 1, 2, \ldots \tag{37}$$

This is a recursive equation whose solution can be found by an iterative procedure. First we focus on the very specific case where j is taken 1 to evaluate the state vector's expectation value. Then we write

$$\begin{aligned}\left\langle \mathbf{s}^{\otimes 1}\right\rangle(t) = \langle \mathbf{s}\rangle(t) &= e^{t\mathbf{E}_{1,1}}\langle \mathbf{s}\rangle(0) + \int_0^t d\tau e^{(t-\tau)\mathbf{E}_{1,1}}\mathbf{E}_{1,2}\left\langle \mathbf{s}^{\otimes 2}\right\rangle(\tau)\\ &= \mathbf{F}(t)\langle \mathbf{s}\rangle(0) + \int_0^t d\tau \mathbf{F}(t-\tau)\mathbf{H}_2\left\langle \mathbf{s}^{\otimes 2}\right\rangle(\tau)\end{aligned} \tag{38}$$

which necessitates the evaluation of the state vector's Kronecker square expectation value. We can use (37) and get

$$\begin{aligned}\left\langle \mathbf{s}^{\otimes 2}\right\rangle(t) &= e^{t\mathbf{E}_{2,2}}\left\langle \mathbf{s}^{\otimes 2}\right\rangle(0) + \int_0^t d\tau e^{(t-\tau)\mathbf{E}_{2,2}}\mathbf{E}_{2,3}\left\langle \mathbf{s}^{\otimes 3}\right\rangle(\tau) = \mathbf{F}(t)^{\otimes 2}\left\langle \mathbf{s}^{\otimes 2}\right\rangle(0)\\ &+ \int_0^t d\tau \mathbf{F}(t-\tau)^{\otimes 2}\left(\mathbf{H}_2 \otimes \mathbf{I}_n + \mathbf{I}_n \otimes \mathbf{H}_2\right)\left\langle \mathbf{s}^{\otimes 3}\right\rangle(\tau)\end{aligned} \tag{39}$$

whose utilization in (38) gives

$$\begin{aligned}\langle \mathbf{s}\rangle(t) = \mathbf{F}(t)\langle \mathbf{s}\rangle(0) &+ \int_0^t d\tau_1 \mathbf{F}(t-\tau_1)\mathbf{H}_2\mathbf{F}(\tau_1)^{\otimes 2}\left\langle \mathbf{s}^{\otimes 2}\right\rangle(0)\\ &+ \int_0^t d\tau_1 \int_0^{\tau_1} d\tau_2 \mathbf{F}(t-\tau_1)\mathbf{H}_2\mathbf{F}(\tau_1-\tau_2)^{\otimes 2}\\ &\times\left(\mathbf{H}_2 \otimes \mathbf{I}_n + \mathbf{I}_n \otimes \mathbf{H}_2\right)\left\langle s^{\otimes 3}\right\rangle(\tau_2)\end{aligned} \tag{40}$$

This equation can also be further iterated by evaluating the state vector's Kronecker cube expectation value to get an expression where the fourth Kronecker power of the state vector appears as the smallest Kronecker power at the right hand side. This produces

$$\begin{aligned}\langle \mathbf{s}\rangle (t) &= \mathbf{F}(t) \langle \mathbf{s}\rangle (0) + \int_0^t d\tau_1 \mathbf{F}(t-\tau_1)\, \mathbf{H}_2 \mathbf{F}(\tau_1)^{\otimes 2} \left\langle \mathbf{s}^{\otimes 2}\right\rangle (0) \\ &+ \int_0^t d\tau_1 \int_0^{\tau_1} d\tau_2 \mathbf{F}(t-\tau_1)\, \mathbf{H}_2 \mathbf{F}(\tau_1-\tau_2)^{\otimes 2} \\ &\times (\mathbf{H}_2 \otimes \mathbf{I}_n + \mathbf{I}_n \otimes \mathbf{H}_2)\, \mathbf{F}(\tau_2)^{\otimes 3} \left\langle s^{\otimes 3}\right\rangle (0) + \cdots \end{aligned} \quad (41)$$

where three central dots stand for the remaining terms involving fourth and higher Kronecker powers of the state vector. Since the matrix **F** depends on its argument exponentially we can write

$$\mathbf{F}(t-\tau_1)\, \mathbf{H}_2 \mathbf{F}(\tau_1)^{\otimes 2} = \mathbf{F}(t)\mathbf{F}(-\tau_1)\mathbf{H}_2 \mathbf{F}(\tau_1)^{\otimes 2} \quad (42)$$

$$\overline{\mathbf{H}}_2(t) \equiv \mathbf{F}(-t)\mathbf{H}_2 \mathbf{F}(t)^{\otimes 2} \quad (43)$$

which urges us to rewrite (41) as follows

$$\begin{aligned}\langle \mathbf{s}\rangle (t) = \mathbf{F}(t) \Bigg\{ &\langle \mathbf{s}\rangle (0) + \int_0^t d\tau_1 \overline{\mathbf{H}}_2(\tau_1) \left\langle \mathbf{s}^{\otimes 2}\right\rangle (0) \\ &+ \int_0^t d\tau_1 \overline{\mathbf{H}}_2(\tau_1) \int_0^{\tau_1} d\tau_2 \left[\mathbf{I}_n \otimes \overline{\mathbf{H}}_2(\tau_2) + \overline{\mathbf{H}}_2(\tau_2) \otimes \mathbf{I}_n \right] \left\langle s^{\otimes 3}\right\rangle (0) + \cdots \Bigg\}\end{aligned} \quad (44)$$

and therefore to define

$$\mathcal{I}_j(t)\mathbf{M}(t) \equiv \int_0^t d\tau \left[\sum_{k=0}^{j-1} \mathbf{I}_n^{\otimes k} \otimes \overline{\mathbf{H}}_2(\tau) \otimes \mathbf{I}_n^{\otimes (j-1-k)} \right] \mathbf{M}(\tau), \quad j = 1, 2, 3, \ldots \quad (45)$$

where $\mathbf{M}(t)$ is a matrix whose row number is compatible for premultiplication with the matrix kernel of $\mathcal{I}_j$. (45)'s utilization in (44) produces the following more explicit equality where the product of calligraphic $\mathcal{I}$s is assumed to be unity when j becomes zero

$$\langle \mathbf{s}\rangle (t) = \mathbf{F}(t) \left\{ \sum_{j=1}^{\infty} \mathcal{I}_1(t) \ldots \mathcal{I}_{j-1}(t) \left\langle \mathbf{s}^{\otimes j}\right\rangle (0) \right\} \quad (46)$$

whose finite sum truncation from the first terms of series form the truncation approximants.

Now we can use a submultiplicative matrix norm (the norm of a product is equal to or less than the product of the norms of the individual factors in this norm) and write the following inequality from (46)

$$\left\| \langle \mathbf{s} \rangle (t) \right\| \leq \left\| \mathbf{F}(t) \right\| \left\{ \sum_{j=1}^{\infty} \left\| \mathcal{I}_1(t) \ldots \mathcal{I}_{j-1}(t) \right\| \left\| \left\langle \mathbf{s}^{\otimes j} \right\rangle (0) \right\| \right\} \tag{47}$$

which urges us to evaluate the norms of matrix integrals $\mathcal{I}$s. If the norm under consideration is chosen in such a way that the norm of the unit matrix takes the value of 1 then it is not hard to see that

$$\left\| \sum_{k=0}^{j-1} \mathbf{I}_n^{\otimes k} \otimes \overline{\mathbf{H}}_2(\tau) \otimes \mathbf{I}_n^{\otimes (j-1-k)} \right\| \leq j \left\| \overline{\mathbf{H}}_2(\tau) \right\|, \quad j = 1, 2, 3, \ldots \tag{48}$$

which enables us to write

$$\left\| \mathcal{I}_1(t) \ldots \mathcal{I}_j(t) \right\| \leq \left(\int_0^t d\tau \left\| \overline{\mathbf{H}}_2(\tau) \right\| \right)^j, \quad j = 1, 2, 3, \ldots \tag{49}$$

and therefore to rewrite (47) as follows

$$\left\| \langle \mathbf{s} \rangle (t) \right\| \leq \left\| \mathbf{F}(t) \right\| \sum_{j=1}^{\infty} \left(\int_0^t d\tau \left\| \overline{\mathbf{H}}_2(\tau) \right\| \right)^{j-1} \left\| \left\langle \mathbf{s}^{\otimes j} \right\rangle (0) \right\| \tag{50}$$

Now we are at a point to use fluctuationlessness theorem which dictates us that the matrix representation of a function operator over a basis set involving a finite number of basis function is equal to the image of the independent variable matrix representations under the function of the function operator when all mathematical fluctuations are ignored. This theorem was first conjectured and proven by Metin Demiralp while its multivariate counterpart has also been conjectured and proven a little bit later by the same author. This theorem remains valid for the Kronecker power expectation values as long as the initial waveform for the expectation value evaluation is appropriately chosen. In this context, we can state the fluctuationlessness theorem for a Kronecker power of state vector as follows: the expectation value of a Kronecker power of the state vector is equal to the same Kronecker power of the state vector's expectation value evaluated via an eigenfunction (which are common for all) of the independent variable matrix representation when all fluctuations are ignored. This can be mathematically expressed as follows

$$\left\langle \mathbf{s}^{\otimes j} \right\rangle_k (0) = \langle \mathbf{s} \rangle_k (0)^{\otimes j}, \quad k = 1, 2, 3, \ldots, N_n \tag{51}$$

where subindex k denotes the fact that expectation value is evaluated with respect to the kth eigenfunction of the universal matrices corresponding n dimensional subspace in the Hilbert space of the multivariate functions which are square integrable. (51) takes us to the following approximation in norm

$$\left\| \left\langle \mathbf{s}^{\otimes j} \right\rangle_k (0) \right\| = \left\| \langle \mathbf{s} \rangle_k (0) \right\|^{\otimes j}, \quad k = 1, 2, 3, \ldots, N_n \tag{52}$$

which urges us to rewrite (50)

$$\| \langle \mathbf{s} \rangle (t) \| \leq \| \mathbf{F}(t) \| \sum_{j=1}^{\infty} \left(\int_0^t d\tau \left\| \overline{\mathbf{H}}_2 (\tau) \right\| \right)^{j-1} \| \langle \mathbf{s} \rangle (0) \|^{\otimes j}. \tag{53}$$

This result implies that the following inequality should be satisfied to get convergence in the truncation approximants

$$\int_0^t d\tau \left\| \overline{\mathbf{H}}_2 (\tau) \right\| \| \langle \mathbf{s} \rangle (0) \| < 1 \tag{54}$$

which completes our convergence analysis on the truncation approximants.

The above convergence condition depends on two entities: (1) The time integral of matrix norm for $\mathbf{H}_2(t)$, which may be considered as a global norm not only on matrix structure but time variation of the relevant entity, (2) The matrix norm of the initial expectation value of the state vector. The former one defines the disk in which the state vector resides. Its value is determined by the expansion point and the commutator of the system's Hamiltonian operator with the state vector whose elements are operators. The state vector is defined in accordance with the expansion point of the Kronecker power expansion. Hence the change of the expansion point causes changes in $\mathbf{H}$ coefficients and therefore in the matrix $\mathbf{F}(t)$ and at the end in $\overline{\mathbf{H}}_2(t)$. This mean the change in the location and the radius in the convergence disk. So it seems to be possible to change convergence domain and cover all possible cases. However, this is a quite comprehensive issue and we do not intend to focus on it here.

8 Evaluating any given analytic operator's expected value

We are now ready to evaluate the expectation value of a given operator $\widehat{O}(\mathbf{s})$. We assume that this operator has the following expression in Kronecker powers of the state vector

$$\widehat{O} (\mathbf{s}) = \sum_{j=0}^{\infty} \mathbf{o}_j^T \mathbf{s}^{\otimes j} \tag{55}$$

where $\mathbf{o}_j$ is a vector of n^j elements. This expression is written by following the inspiration from the analytic functions. Hence, we call any operator, which can be expressed in this manner, "analytic". (55) allows us to write the following equation as long as the series at its right hand side converges.

$$\left\langle \widehat{O}\left(\mathbf{s}\right)\right\rangle(t)=\sum_{j=0}^{\infty}\mathbf{o}_j^T\left\langle \mathbf{s}^{\otimes j}\right\rangle(t) \tag{56}$$

whose right hand side expected value can be taken from the solution of the probabilistic evolution equation. If we define

$$\mathbf{o}_{coef}\equiv\left[\,\mathbf{o}_0^T\ \mathbf{o}_1^T\ \ldots\ \right]^T \tag{57}$$

then we can rewrite (56) in the following concise form

$$\left\langle \widehat{O}\left(\mathbf{s}\right)\right\rangle(t)=\mathbf{o}_{coef}^T\boldsymbol{\xi}(t). \tag{58}$$

This is the final form of the expected value for a given analytic operator.

9 Conclusion

In this work we have brought a new perspective to quantum dynamical problems. The approach does not explicitly use the Schrödinger equation and the wave function whose initial form is the only required entity. The purpose is to get ODE(s) with initial conditions and this could be accomplished by using the expectation values which are the ultimate targets to be evaluated in fact. The use of state vector whose elements are the operators characterizing the system under consideration, and, its nonnegative outerpowers are used as the basis entities and their expectation values served to construct an infinite set of ODEs with appropriate initial conditions.

Here, the mainlines of the theory and basic concepts are given. The convergence of the truncation approximants have also been investigated. A rather simple inequality has been found to define the convergence domain for the state vector's initial expectation norm. Practical applications will be the topic of our future works. We list a few important publications of the author and his group in the references together with certain rather recent important resources on ODEs for further reading since they are the only basic references at this moment. The references [1–4] are about the PEA while [5–9] are related to mathematical fluctuations whereas [10–14] are for certain important resources published rather recently.

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